Class 4: CISD, CCSD and basic DFT

1. Use rdesktop to login to the Windows Terminal Server at minsc.oerc.ox.ac.uk (use your supercomputer login credentials).

2. Use ssh from either the Linux host or from the terminal server to login to orac.oerc.ox.ac.uk and load the Gaussian module (module load gaussian03).

3. Optimize the geometry of methane at MP2/cc-pVDZ level and compute the energy at the minimum using MP2, MP4, CISD(T), CCSD and CCSD(T) methods. Use scf=dsymm to enforce the use of tetrahedral symmetry, otherwise the calculation may take a long time.

4. Optimize glucose geometry using DFT B3LYP/6-31G(d,p) method. Observe the time taken.

5. Compare the hyperfine couplings computed for phenyl neutral radical (benzene without one hydrogen) using RB3LYP/cc-pVDZ, UB3LYP/cc-pVDZ and UB3LYP/EPR-II methods. Comment on the results and compare them to experimental data.

6. Use the redundant coordinate editor in GaussView to set up a potential energy scan with respect to the C-H bond stretch in methane (between 1 and 4 Angstroms). Run the scan using RHF, UHF, RMP2, UMP2, RCCSD, UCCSD, RB3LYP and UB3LYP methods in a cc-pVDZ basis set. Read the logs with GaussView and plot the molecular energy against the stretch parameter. Comment on what you see.

Reminder: ORAC runscripts should look like this

```bash
#!/bin/bash
#PBS -l ncpus=8
#PBS -l walltime=24:00:00
#PBS -V

cd $PBS_O_WORKDIR
GAUSS_SCRDIR=$TMPDIR
export GAUSS_SCRDIR

g03 ******.com
g03 ******.com
g03 ******.com
```